

Face-centred cubic lattices and particle redistribution in vortex methods[†]

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Abstract. In vortex particle methods one is concerned with the problem of clustering and depletion of particles in different regions of the flow. The overlap of the vortex blobs is indeed of primary importance for the convergence of the method. In this paper we consider face-centred cubic (FCC) lattices for particle redistribution in three dimensions. This lattice is in fact the most natural way to pack spheres (the FCC is also known as a *closest-sphere packing* lattice). As a consequence, a point has 12 equidistant close neighbours rather than six for the cubic lattice. The FCC lattice thus offers some symmetry properties that should prove useful for a number of reasons, e.g., the core overlap issue. A few results for this scheme are presented. The problem of two colliding vortex rings at $Re = 250$ and 500 is studied with both the FCC and cubic lattice schemes. This problem subjects the vortex tubes to a quite strong stretching field and can amply test the quality of the lattice and the remeshing.

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1. Introduction

Vortex particle methods are based on the representation of the vorticity by a set of Lagrangian elements. The quality of this representation is critical for the convergence of the method. Because they are Lagrangian, the vortex elements can rapidly cluster along principal axes of compression and form gaps along axes of extension.

Two very different approaches to maintain an approximately uniform distribution stand out. In one, the particles are split or merge depending on the flow locally [1]–[3]. This usually results in a non-controlled growth of the number of particles. Another method consists in redistributing particles onto a regular lattice. A number of schemes have been proposed (see [4] for a review). They are usually designed to conserve the first moments of the particle distribution and/or to distribute the new vorticity field smoothly onto the new points.

These families of schemes are normally based on a regular cubic lattice; they are built in one dimension at first and their extension to two and three dimensions is straightforward by use of a tensor product. These schemes have been used with a spatially varying resolution but even so they are still based on a cubic lattice [5]–[7].

In this work, we introduce a new family of schemes based on the *face-centred cubic* (FCC) lattice. It is also called a *closest-sphere packing* lattice because it is in fact the natural way to pack spheres. The motivation for this work is that this lattice is naturally closer to the spherical nature of the particles. For example, in flows with a boundary, it also may be helpful to have an isotropic cloud of particles near the wall to reduce noise in quantities measured at the wall.

This paper is organized in the following manner: the incompressible flow equations are presented first, with the vortex method, the FCC lattice and particle redistribution, the results and the conclusion following.

2. Three-dimensional incompressible flow

We solve the vorticity equation for an incompressible flow in an unbounded domain:

$$\frac{D\boldsymbol{\omega}}{Dt} = (\nabla \mathbf{u}) \cdot \boldsymbol{\omega} + \nu \nabla^2 \boldsymbol{\omega} \quad (1)$$

$$\nabla \cdot \mathbf{u} = 0 \quad (2)$$

where $\mathbf{u}(\mathbf{x}, t)$ is the velocity field, ν is the kinematic viscosity and $\boldsymbol{\omega} = \nabla \times \mathbf{u}$ is the vorticity.

A Helmholtz decomposition is used to determine the velocity:

$$\mathbf{u} = \nabla \phi + \nabla \times \boldsymbol{\psi} \quad (3)$$

with $\nabla \cdot \boldsymbol{\psi} = 0$. Here ϕ is a scalar potential and the corresponding velocity is irrotational. $\boldsymbol{\psi}$ is the streamfunction which is related to the vorticity by the Poisson equation:

$$\nabla^2 \boldsymbol{\psi} = -\boldsymbol{\omega}. \quad (4)$$

3. Vortex method

The vortex method is based on the representation of the vorticity field by a set of N Lagrangian particles:

$$\tilde{\omega}(\mathbf{x}, t) = \sum_{i=1}^N \zeta_i(\mathbf{x} - \mathbf{x}_i) \alpha_i. \quad (5)$$

The particles have a position \mathbf{x}_i and a strength $\alpha_i = \int \omega \, d\mathbf{x}$. The streamfunction, the velocity and its gradient can be computed by means of a Green function. This Green function is associated with the kernel used to represent the particles. One then uses the velocity and its gradient to move the particles and update their strengths, respectively.

The basis used to represent the vorticity field is not necessarily divergence free whereas $\omega = \nabla \times \mathbf{u}$ is clearly solenoidal. This second field allows the design of some relaxation methods for $\tilde{\omega}$ [8, 9] and allows the monitoring of the divergence error defined by

$$E_{div} = \int |\tilde{\omega} - \omega|^2 \, d\mathbf{x}. \quad (6)$$

This divergence problem can be alleviated by a certain choice of the numerical evaluation of the stretching term in equation (1) [4].

4. Particle redistribution

As mentioned above, the vortex particle method is subject to problems of clustering and depletion. A solution consists in creating a new set of particles on a regular lattice. This is called particle redistribution. This process is characterized by the order of the highest conserved moment, the width of the stencil (i.e. how many particles are generated for one particle of the old set) and the smoothness of the interpolation function used.

It is worth noting that the redistribution scheme can also help reduce the divergence error. The particle pattern influences the quality of the particle interactions; these interactions at close range play an important role when one computes the velocity and its gradient and also when a viscous scheme is used.

A more thorough discussion can be found in [4, 7].

4.1. The face-centred cubic lattice

The cubic lattice has been so far the only lattice used for these redistributions. The vortex element method is a grid-free method (with the exception of the redistribution); the geometrical pattern of the particles therefore should not have any influence on the convergence of the method provided the pattern is regular.

The FCC lattice offers such a regularity and also some interesting symmetry properties. This lattice is known as a *closest-sphere packing* lattice; it is one of two lattices that pack the most spheres per unit volume (the other one is the *hexagonal close-packing* (HCP) lattice). We chose the FCC because it is possible to fit a coordinate system that is very helpful in the design of the scheme. A node of this lattice has 12 equidistant direct neighbours against six for a cubic lattice and there are four planes with a mesh parameter h passing through a node (three for a cubic). This lattice is not difficult to generate if one considers it as the superposition of three families of two-dimensional hexagonal lattices, A, B and C in figure 1.

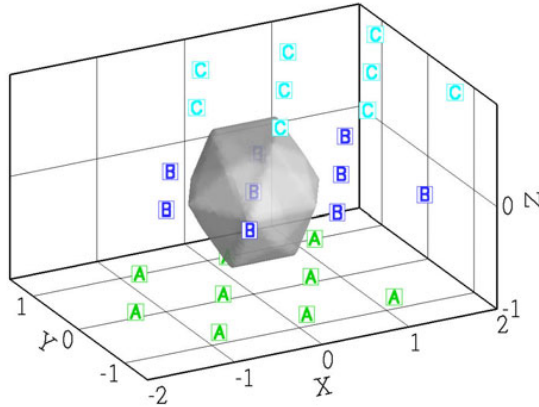


Figure 1. The FCC lattice and the interpolation function: the three families of hexagonal planes used to generate the lattice and the isovolume $W_{FCC_1} = 0.25$.

4.2. The interpolation function

The second component of the redistribution is the interpolation rule W one uses to create the new set of particles,

$$\alpha_p^{new} = \sum_q \alpha_q^{old} W\left(\frac{\mathbf{x}_p - \tilde{\mathbf{x}}_q}{h}\right).$$

For the cubic lattice, several families of schemes have been introduced. The great majority of these are based on the tensor product of one-dimensional interpolation functions. For the FCC lattice, such a construction is not possible; the interpolation function has to be built in three dimensions from the start.

We designed a continuous second order interpolation function that is analogous to the three-dimensional *Witches Hat* Λ_1 function for a cubic lattice. This rule redistributes a particle onto the vertices of the containing tetrahedron or octahedron (four or six points respectively). This function is defined by pieces; it is a linear function inside a tetrahedron and a piecewise linear continuous function inside an octahedron. This function was built to conserve circulation and its first moment and to ensure continuity with the linear function inside the tetrahedra of the stencil. This piecewise definition is visible in the isocontour in figure 1. Analytical expressions and C functions are available at <http://www.galcit.caltech.edu/~philch/research.en.html>.

We call this scheme FCC_1 . Notice that it is straightforward to generate smoother interpolation functions with a wider stencil. The convolution of our scheme by a *closest-point* distribution function yields a scheme with the same moment conservation but with one more level of continuity. Improving the conservation properties takes more work.

5. Results

Our test consists in two colliding vortex rings. This configuration deforms the set of particles and thus tests the quality of the core overlap through the simulation. There are two sets of results. The first one is a well resolved case at $Re = 250$ where we compare two second order schemes, the Λ_1 in the cubic lattice and our FCC_1 scheme. The second set of results is at $Re = 500$ with a coarser resolution (thus under-resolved) and we consider the two second order schemes along with a third order scheme M'_4 . The redistribution frequency (once every ten time steps) was the same in all our tests.

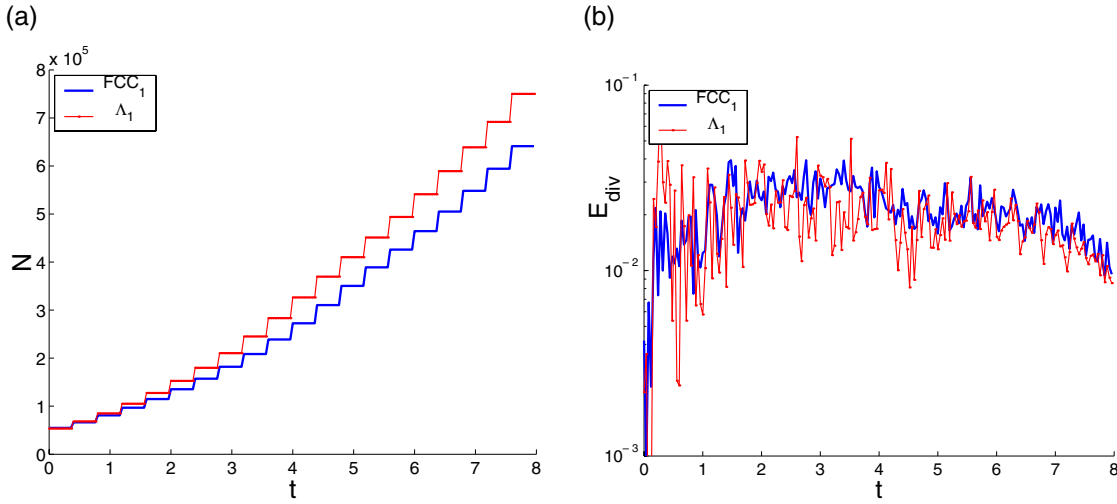


Figure 2. $Re = 250$: number of particles and divergence error.

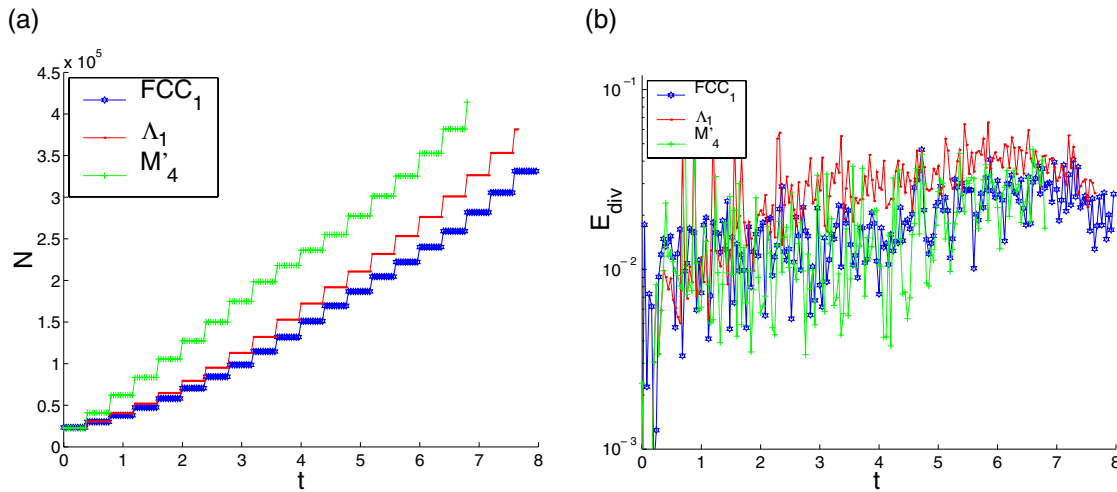


Figure 3. $Re = 500$: number of particles and divergence error.

5.1. $Re = 250$

Because of the different lattices used, we define the grid Reynolds number as $Re_h = \frac{UV_p^{1/3}}{\nu}$. It will depend on the actual density of points. The results in this section were obtained at $Re_h \approx 12 \rightarrow 4$. The FCC lattice introduces fewer points than the Λ_1 scheme and shows the same divergence error (figure 2). The error decreases for $t > 6$ as the rings are decaying.

5.2. $Re = 500$

We now consider the under-resolved case, $Re_h \approx 27 \rightarrow 13$. One can now notice a significant difference between the two second order schemes. The error for the FCC_1 scheme stays at the level of the M'_4 which introduces far more particles because of its wider stencil (figure 3).

6. Conclusion

We have introduced the first representative of a new family of interpolation schemes based on the FCC lattice. Our scheme has two outstanding features.

- (i) Thanks to the many symmetries of the FCC lattice, it is more compact than an equivalent scheme in a cubic lattice. This results in a slower growth of the number of particles because of a tighter *halo* of new particles around the set of old particles.
- (ii) Symmetry is also beneficial to the overlap of the particle cores and allows better communications between the particles even under stretching. We have observed a significant effect in the divergence error for high Re_h cases.

Acknowledgment

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